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Mesoscopic to universal crossover of transmission phase of multi-level quantum dots

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Transmission phase α measurements of many-electron quantum dots (small mean level spacing δ) revealed universal phase lapses by π between consecutive resonances. In contrast, for dots with only a few electrons (large δ), the appearance or not of a phase lapse depends on the dot parameters. We show that a model of a multi-level quantum dot with local Coulomb interactions and arbitrary level-lead couplings reproduces the generic features of the observed behavior. The universal behavior of α for small δ follows from Fano-type antiresonances of the renormalized single-particle levels.

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One of the longest-standing puzzles in mesoscopic physics is the intriguing phase-lapse behavior observed in a series of experiments [1, 2, 3] on Aharonov-Bohm rings containing a quantum dot in one arm. Under suitable conditions in linear response, both the phase and magnitude of the transmission amplitude $T = |T|e^{i\alpha}$ of the dot can be extracted from the Aharonov-Bohm oscillations of the current through the ring. If this is done as function of a plunger gate voltage V_g that linearly shifts the dot's single-particle energy levels downward, $\varepsilon_j = \varepsilon_j^0 - V_g$ ($j = 1, 2, \ldots$ is a level index), a series of well-separated transmission resonances [peaks in $|T(V_g)|$, to be called "Coulomb blockade" (CB) peaks] of rather similar width and height was observed, across which $\alpha(V_g)$ continuously increased by π, as expected for Breit-Wigner-like resonances. In each CB valley between any two successive CB peaks, α always jumped sharply downward by π ("phase lapse", PL). The PL behavior was observed to be "universal", occurring in a large succession of valleys for every many-electron dot studied in [1, 2, 3]. This universality is puzzling, since naively the behavior of $\alpha(V_g)$ is expected to be "mesoscopic", *i.e.* to show a PL in some CB valleys and none in others, depending on the dot's shape, the parity of its orbital wavefunctions, etc. Despite a large amount of theoretical work (reviewed in [4, 5]), no fully satisfactory framework for understanding the universality of the PL behavior has been found yet.

A hint at the resolution of this puzzle is provided by the most recent experiment [3], which also probed the few-electron regime: as V_g was increased to successively fill up the dot with electrons, starting from electron number $N_e = 0$, $\alpha(V_g)$ was observed to behave mesoscopically in the *few*-electron regime, whereas the above-mentioned universal PL behavior emerged only in the *many*-electron regime ($N_e \gtrsim 15$). Now, one generic difference between few- and many-electron dots is that the latter have smaller level spacings $\delta_j = \varepsilon_{j+1}^0 - \varepsilon_j^0$ for the topmost filled levels. With increasing N_e, their δ_j's should eventually become smaller than the respective level widths Γ_j stemming from hybridization with the leads. Thus, Ref. 3 suggested that a key element for understanding the universal PL behavior might be that *several overlapping single-particle levels simultaneously* contribute to transport. Due to the dot's Coulomb charging energy U, the transmission peaks remain well separated nevertheless.

Previous works have studied the transmission amplitude of multi-level, interacting dots [6, 7, 8, 9, 10]. However, no systematic study has yet been performed of the interplay of level spacing, level widths, and charging energy that combines a wide range of parameter choices with an accurate treatment of the correlation effects induced by the Coulomb interaction. The present Letter aims to fill this gap by using two powerful methods, the numerical (NRG) [11, 12] and functional (fRG) [13] renormalization group approaches, to study systems with up to 4 levels (for spinless electrons; see below). We find that if the ratio of average level spacing δ to average level width Γ is decreased into the regime $\delta \lesssim \Gamma$, one of the *renormalized effective single-particle levels generically* becomes wider than all others, and hovers in the vicinity of the chemical potential μ in the regime of V_g for which the PLs occur. Upon varying V_g, the narrow levels cross μ *and* the broad level, leading to Fano-type antiresonances accompanied by universal PLs. For $\delta \gtrsim \Gamma$, $\alpha(V_g)$ behaves mesoscopically [14] for all U. Decreasing δ thus causes the PL behavior to generically change from mesoscopic to universal, as observed experimentally [3].

Model: The dot part of our model Hamiltonian is

$$H_{\mathrm{dot}} = \sum_{j=1}^{N} \varepsilon_j n_j + \frac{1}{2} U \sum_{j \neq j'} \left(n_j - \tfrac{1}{2}\right)\left(n_{j'} - \tfrac{1}{2}\right) ,$$

with $n_j = d_j^\dagger d_j$ and dot creation operators $d_j^\dagger$ for spinless electrons, where $U > 0$ describes Coulomb repulsion. The semi-infinite leads are modeled by a tight-binding chain $H_l = -t \sum_{m=0}^{\infty} (c_{m,l}^\dagger c_{m+1,l} + \mathrm{H.c.})$ and the level-lead couplings by $H_T = -\sum_{j,l} (t_j^l c_{0,l}^\dagger d_j + \mathrm{H.c.})$, where $c_{m,l}$ annihilates an electron on site m of lead $l = L, R$ and

t_j^l are real level-lead hopping matrix elements. Their relative signs for successive levels, $s_j = \mathrm{sgn}(t_j^L t_j^R t_{j+1}^L t_{j+1}^R)$, are sample-dependent random variables determined by the parity of the dot's orbital wave functions. The effective width of level j is given by $\Gamma_j = \Gamma_j^L + \Gamma_j^R$, with $\Gamma_j^l = \pi\rho|t_j^l|^2$. We take ρ, the local density of states at the end of the leads, to be energy independent, choose $\mu = 0$, and specify our choices of t_j^l using the notation $\sigma = \{s_1, s_2, \ldots\}$, $\gamma = \{\Gamma_1^L, \Gamma_1^R, \Gamma_2^L, \ldots\}$, $\Gamma = \frac{1}{N}\sum_{j,l}\Gamma_j^l$.

Methods: We focus on linear response transport and unless stated otherwise, on zero temperature ($\tau = 0$). Then the dot produces purely elastic, potential scattering between left and right lead, characterized by the transmission matrix $T_{ll'} = 2\pi\rho\sum_{ij} t_i^l \mathcal{G}_{ij}^R(0) t_j^{l'}$, where $\mathcal{G}_{ij}^R(\omega)$ is the retarded local Green function which we compute using NRG and fRG. The NRG is a numerically exact method that is known to produce very accurate results [11, 12]. The fRG is a renormalization procedure for the self-energy Σ and higher order vertex functions (see [13] for details). We use a truncation scheme that keeps the flow equations for Σ and for the frequency independent part of the effective two-particle (Coulomb) interaction. Comparisons with NRG [13] have shown this approximation to be reliable provided that the number of (almost) degenerate levels and the interaction do not become too large. fRG is much cheaper computationally than NRG, enabling us to efficiently explore the vast parameter space relevant for multi-level dot models.

At the end of the fRG flow, the full Green function at zero frequency takes the form $[\mathcal{G}^R(0)]_{ij}^{-1} = -h_{ij} + i\Delta_{ij}$, with an effective, *noninteracting* (but V_g *and* U-dependent) single-particle Hamiltonian $h_{ij} = (\varepsilon_j^0 - V_g)\delta_{ij} + \Sigma_{ij}$, whose level widths are governed by $\Delta_{ij} = \pi\rho\sum_l t_i^l t_j^l$. To interpret our results, we adopt the eigenbasis of $[\mathcal{G}^R(0)]_{ij}^{-1}$, with eigenvalues $-\tilde{\varepsilon}_j + i\tilde{\Gamma}_j$, and view $\tilde{\varepsilon}_j$ and $\tilde{\Gamma}_j$ as level positions and widths of a renormalized effective model (REM) describing the system.

For LR-symmetry, $\Gamma_j^L = \Gamma_j^R$, an NRG-shortcut can be used, which is much less demanding than computing the full $G_{ij}^R(\omega)$: the S-matrix is then diagonal in the even-odd basis of the leads and its eigenvalues depend on the total occupancies $n_\pm$ of all levels coupled to the even/odd lead (Friedel sum rule), so that the transmission amplitude $T = T_{LR}$ takes the form $T = \sin[\pi(n_+ - n_-)]e^{i\pi(n_+ + n_-)}$. A transmission zero (TZ) and hence PL occurs when $n_+ = n_- \bmod 1$ [Figs. 1(e,h): $n_\pm$ in thin dashed/dashed-dotted line].

Results: Our results are illustrated in Figs. 1 to 3. fRG and NRG data generally coincide rather well (compare black and orange lines in Figs. 1 and 2), except for $N = 4$ when both $U \gg \Gamma$, $\delta < \Gamma$, and correlations become very strong [Fig. 2(f)]. The figures show the following striking qualitative features, that we found to be generic by running the fRG for ten-thousands of parameter sets, which is possible as a complete $T(V_g)$ curve can be obtained within a few minutes on a standard PC:

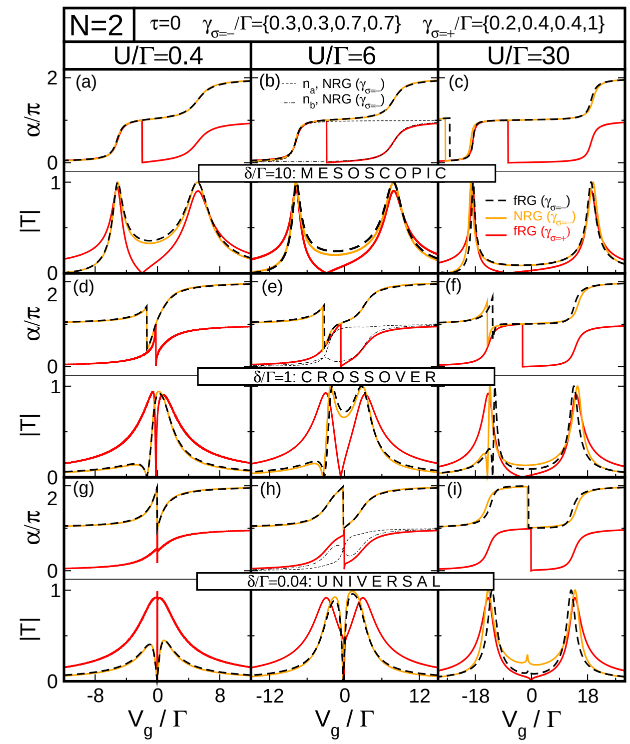

FIG. 1: $|T(V_g)|$ and $\alpha(V_g)$ for $N = 2$, $\varepsilon_{2,1}^0 = \pm\delta/2$, and $\tau = 0$: decreasing δ/Γ produces a change from (a,b,c) mesoscopic via (d,e,f) crossover to (g,h,i) universal behavior; increasing U/Γ leads to increased transmission peak spacing. (b,e,h) include the occupancies n_+ (thin dashed) and n_- (thin dash-dotted) of the levels coupled to the even/odd lead in the case of LR-symmetry. The condition $n_+ = n_- \bmod 1$ produces a TZ and PL. For the blip and hidden TZ near $V_g = 0$ in (i), see [15].

Mesoscopic regime: For $\delta \gtrsim \Gamma$ [Figs. 1(a,b,c), 2(a,b,c)], we recover behavior that is similar to the $U = 0$ case. Within the REM it can be understood as transport occurring through only one effective level at a time [see Fig. 3(a,b,c)], with $\tilde{\Gamma}_j \simeq \Gamma_j$. Each $\tilde{\varepsilon}_j$ that crosses μ produces a Breit-Wigner-like transmission resonance of width $2\Gamma_j$ and height governed by Γ_j^L/Γ_j^R. At the crossing the other levels are shifted upwards by U [charging effect; Fig. 3(a)] leading to renormalized peak separations ("level spacings") $\delta_j + U$. Between two peaks, $\alpha(V_g)$ behaves mesoscopically: depending on the sign s_j one either observes a PL ($s_j = +$) or continuous evolution of α ($s_j = -$) [14]. Additional PLs occur to the left or right, beyond the last transmission peak [Fig. 2(a)].

Mesoscopic to universal crossover: As the ratio δ/Γ is reduced, the behavior changes dramatically: the TZs and PLs that used to be on the far outside move inward across CB resonances [see evolution in Figs. 1(b,e,h)].

Universal regime: A universal feature [16] emerges for $\delta \lesssim \Gamma \lesssim U$ (crossover scales are of order 1, but depend on the chosen parameters): for *all* choices of the signs σ and generic couplings γ, the N CB peaks over which α increases by π *are separated by* $N-1$ *PLs,* each accompanied by a TZ [Figs. 1(g,h,i), 2(d,e,f)]. This is consis-

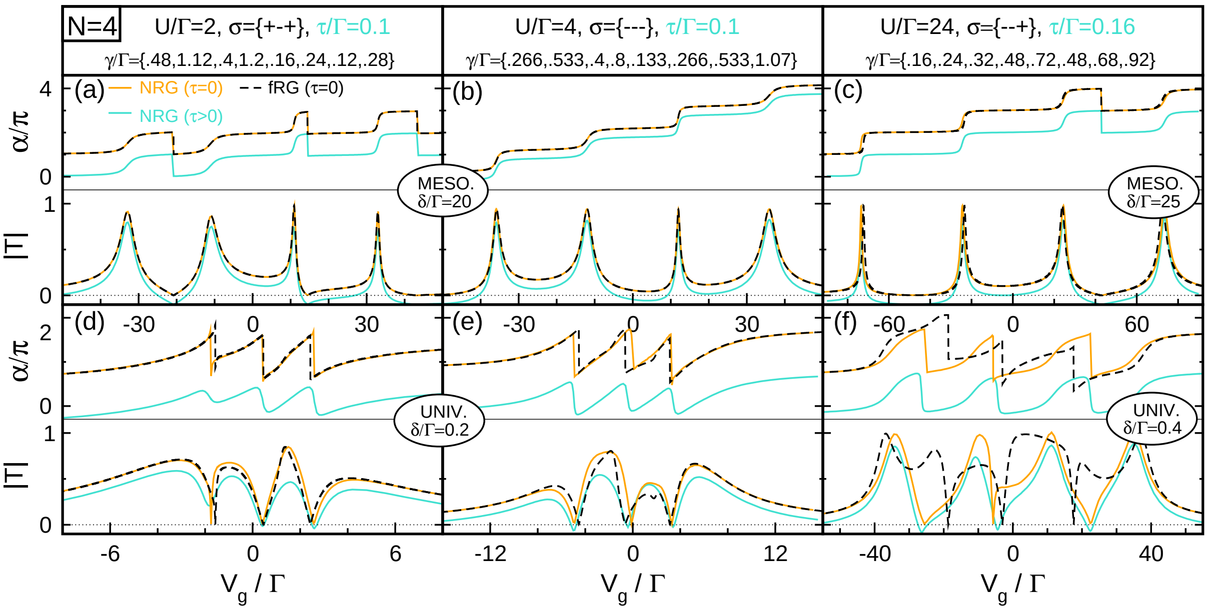

FIG. 2: $|T(V_g)|$ and $\alpha(V_g)$ for $N=4$, with equidistant levels, $\delta_j \equiv \delta$. The qualitative features do not change if this assumption is relaxed, or if U is assumed to be slightly level-dependent, $U \to U_{jj'}$. Decreasing δ/Γ produces a crossover from (a,b,c) mesoscopic to (d,e,f) universal behavior; increasing U/Γ leads to increased spacing of the transmission peaks and PLs. For clarity the finite temperature ($\tau > 0$) curves were shifted downwards (by 0.1 for $|T|$). (f) For $U/\Gamma \gg 1$ and $\tau/\Gamma = 0.16$, the CB peak and PL shapes are strikingly similar to those observed experimentally at comparable ratios of τ/Γ (see Fig. 3 of [2] and Fig. 6 of [3]). For small δ/Γ *and* $U/\Gamma \gg 1$ fRG becomes less reliable and the results begin to differ from those of NRG.

tent with the experimentally observed trend. For small to intermediate values of U/Γ [Figs. 1(g,h), 2(d,e)], the transmission peaks are not well-separated, and $\alpha(V_g)$ has a saw-tooth shape. As U/Γ increases so does the peak separation and the corresponding phase rises take a more S-like form [Figs. 1(h,i), 2(e,f)]. At finite temperatures of order $\tau \gtrsim \delta$ [17] sharp features are smeared out (Fig. 2). For U/Γ as large as in Figs. 1(i) and 2(f), the behavior of $\alpha(V_g)$ (both the S-like rises and the universal occurrence of PLs in each valley) as well as the one of $|T(V_g)|$ (similar width and height of all CB peaks) is very reminiscent of that observed experimentally, in particular for $\tau \gtrsim \delta$ [Fig. 2(f)]. For $U/\Gamma \gg 1$ the full width of the CB peaks is of order $2N\Gamma$ (not $2\Gamma_j$ as in the mesoscopic regime), indicating that several bare single-particle levels simultaneously contribute to transport. The τ dependence of the width of the PLs is different from the behavior $\tau^2/(\delta+U)^2$ found in the mesoscopic regime [19] and will be discussed in an upcomming publication. Note that for the temperatures considered here the width of the PLs is still much smaller than the width of the CB peaks.

For certain fine-tuned parameters (γ and σ) the behavior at small δ/Γ deviates from the generic case. For $N = 2$ the nongeneric cases were classified in [9]. In Fig. 1 only generic parameters are shown. For $N \geq 3$ LR-symmetric couplings produce nongeneric features. However, these features are irrelevant to the experiments. They quickly disappear upon switching on LR-asymmetry or $\tau > 0$.

Interpretation: We can gain deeper insight into the appearance of the TZs and PLs in the universal regime from the properties of the REM obtained by fRG for moderate U/Γ [at which NRG and fRG agree well; Fig. 2(b,e)]. For $N \geq 3$, $\delta \lesssim \Gamma$ and $U = 0$, two of the effective levels are much wider than the others, since Δ_{ij}, being a matrix of rank 2, has only two nonzero eigenvalues [18] (for the $N = 2$ case, see [16, 19]). We found that this also holds at $U > 0$: for $N = 3, 4$ one effective level is typically a factor of 2 to 3 wider than the second widest, while the remaining 1 or 2 levels are very narrow [Fig. 3(f)]. At $\delta \lesssim \Gamma$ [Fig. 3(d)] the *interaction* leads to a highly nonmonotonic dependence of $\tilde{\varepsilon}_j$ on V_g which is essential for our universal PL scenario: As V_g is swept, the widest level hovers in the vicinity of μ over an extended range of V_g values, whereas the narrow ones cross μ – and therefore also the widest one – rather rapidly. This leads to a Fano-type effect [20, 21, 22, 23, 24] whose effective Fano parameter q is real, by time-reversal symmetry [21]. Thus, each TZ, and hence PL, can be understood as a Fano-type antiresonance arising (irrespective of the signs of t_i^l) from destructive interference between transmission through a wide and a narrow level. The crossings of the narrow levels and μ, and thus the PLs, are separated by U due to charging effects. In contrast, for $U = 0$, $\tilde{\varepsilon}_j \propto -V_g$ for *all* renormalized levels and no levels cross each other. Our fRG studies indicate that for the regime $\delta \lesssim \Gamma$, the Fano-antiresonance mechanism is generic for $U \gtrsim \Gamma$. We thus expect it to apply also for interactions $U \gg \Gamma$ for which fRG is no longer reliable.

The fact that the combination of a wide and several narrow levels leads to PLs was first emphasized in [8] (without reference to Fano physics). However, whereas in [8] a *bare* wide level was introduced as a model assumption (backed by numerical simulations for noninteracting dots of order 100 levels), in our case a *renormalized*

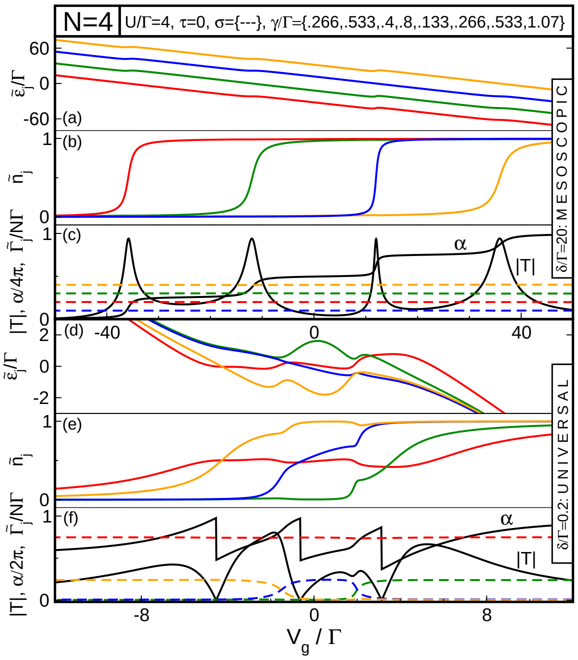

FIG. 3: Renormalized single-particle energies $\tilde{\varepsilon}_j$, occupancies $\tilde{n}_j$ and level widths $\tilde{\Gamma}_j$ (dashed) of the REM, and the resulting $|T|$ and α (all as functions of V_g), for $N = 4$ and $\delta_j \equiv \delta$ at $\tau = 0$. The parameters are the same as in Fig. 2(b,e).

wide level is generated for *generic* couplings if $\delta \lesssim \Gamma$. Also, whereas in [8] the wide level repeatedly empties into narrow ones as V_g is swept (because $\Gamma_{\rm wide} \ll U$ was assumed), this strong occupation inversion [25] is not required in our scenario. In Fig. 3(e), e.g., the wide level remains roughly half-occupied for a large range of V_g, but TZs and PLs occur nevertheless. We thus view occupation inversion, if it occurs, as a side effect, instead of being the cause of PLs [26].

Conclusions: The most striking feature of our results, based on exhaustive scans through parameter space for $N = 2, 3, 4$, is that for any given, generic choice of couplings (γ and σ), the experimentally observed crossover [3] from mesoscopic to universal $\alpha(V_g)$-behavior can be achieved within our model by simply changing the ratio δ/Γ from $\gtrsim 1$ to $\lesssim 1$, provided that $U \gtrsim \Gamma$. The universal π PLs result from Fano-type antiresonances of effective, renormalized levels, which arise because interactions cause a broad level (occuring, if $\delta \lesssim \Gamma$, already for $U = 0$) to be repeatedly crossed by narrow levels. A quantitative description requires correlations to be treated accurately. We expect that the main features of this mechanism carry over to the case of spinful electrons, since for $\delta \lesssim \Gamma$ spin correlation physics (such as the Kondo effect) does not play a prominent role [27].

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[15] For $N = 2$, U larger than a critical value and in the limit $\delta \to 0$, two additional, sharp peaks appear on both sides of the TZ and exponentially close to it (peaks and TZ are visible only as a blip in Fig. 1(i), due to lack of resolution) [9]. Similar sharp features occur for $N > 2$, see Fig. 2(f). These features, which get smeared out with increasing temperature, are irrelevant for the PL puzzle.
[16] For $\delta \lesssim \Gamma$, generic Γ_j^l and $N = 2$, the universal PL behavior (1 PL between the 2 CB peaks) already occurs at $U = 0$. For $N > 2$ and small U/Γ, universal behavior ($N - 1$ PL between N CB peaks) sets in only once U/Γ becomes large enough.
[17] For $\tau > 0$, we calculate $|T|e^{i\alpha} \equiv -\int d\varepsilon \partial_\varepsilon f(\varepsilon) T^\tau_{\rm LR}(\varepsilon)$ [7, 19], where the finite-temperature transmission matrix T^τ is obtained via the full density matrix NRG of [12].
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[26] In a model with a weakly V_g-dependent, bare wide level and several narrow levels with $\delta > \Gamma$, Fano-like interference produces TZs and PLs even at $U = 0$, for which interaction-induced occupation inversions are absent [24].
[27] We have recently shown this explicitly for $N = 2$ [19].